PTO-1590 (8-01)

Kathlen Fuller

Access DB# 160064

#### **SEARCH REQUEST FORM**

Scientific and Technical Information Center

Requester's Full Name: Examiner #: Phone Number 30 Art Unit: Serial Number: Mail Box and Bldg/Room Location: Results Format Preferred (circle): #APER DISK If more than one search is submitted, please prioritize searches in order of need. Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc. if known. Please attach a copy of the cover sheet, pertinent claims, and abstract. Title of Invention: Inventors (please provide full names): Earliest Priority Filing Date: \*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the Could you have to a Cell Confrig a phospholic denuiting of Formula (2) wherein Rack Ry weth Mon water Substitut or a holigen element when at last one of R' is a hologin clemn 3=n=15. Se p26 (atoch) to defrom R" If Can And above Please Hen Sieve truter Cell Compressing an electrolyte Comprising Phospharene **STAFF USE ONLY** Type of Search Vendors and cost where applicable NA Sequence (#) STN Searcher Phone #: AA Sequence (#) Searcher Location: Questel/Orbit Structure (#) Date Searcher Picked Up Bibliographic Dr.Link Date Completed: Litigation Lexis/Nexis Searcher Prep & Review Time: Sequence Systems Fulltext Clerical Prep Time: Patent Family WWW/Internet Online Time: Other (specify)



# STIC Search Report

#### STIC Database Tracking Number: 160084

TO: Laura Weiner Location: 6C83 Art Unit: 1745 August 10, 2005

Case Serial Number: 10048054

From: Kathleen Fuller Location: EIC 1700 REMSEN 4B28

Phone: 571/272-2505

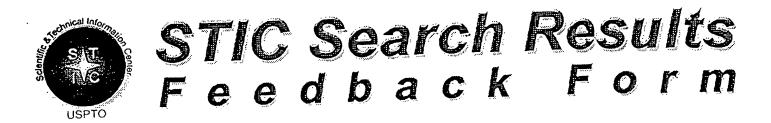
Kathleen.Fuller@uspto.gov

#### Search Notes

were 187 structures but none with utility. I printed out 2 answers where there were 3-15 phosphorus per the claims-none on utility.

I searched the formula 1 first; there are some good answers. Then I realized you wanted formula 2. There





## EC17000

Questions about the scope or the results of the search? Contact the EIC searcher or contact:

Kathleen Fuller, EIC 1700 Team Leader 571/272-2505 REMSEN 4B28

Voluntary Results Feedback Form
<ul> <li>I am an examiner in Workgroup: Example: 1713</li> <li>Relevant prior art found, search results used as follows:</li> </ul>
<ul><li>102 rejection</li><li>103 rejection</li></ul>
<ul> <li>Cited as being of interest.</li> <li>Helped examiner better understand the invention.</li> <li>Helped examiner better understand the state of the art in their technology.</li> </ul>
Types of relevant prior art found:  [ Foreign Patent(s)  [ Non-Patent Literature       (journal articles, conference proceedings, new product announcements etc.)
<ul> <li>Relevant prior art not found:</li> <li>Results verified the lack of relevant prior art (helped determine patentability).</li> <li>Results were not useful in determining patentability or understanding the invention.</li> </ul>
Comments:

WEINER 10/936148 08/10/2005

RPage 1

=> file req

FILE 'REGISTRY' ENTERED AT 11:19:04 ON 10 AUG 2005
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 AUG 2005 HIGHEST RN 859282-03-4 DICTIONARY FILE UPDATES: 9 AUG 2005 HIGHEST RN 859282-03-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> file hcaplus

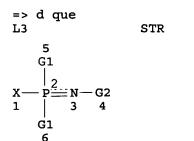
FILE 'HCAPLUS' ENTERED AT 11:19:08 ON 10 AUG 2005
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 10 Aug 2005 VOL 143 ISS 7 FILE LAST UPDATED: 9 Aug 2005 (20050809/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.



1,582 structures from this query formula I

VAR G1=A/X VAR G2=C/SI/GE/SN/N/P/AS/SB/BI/O/S/SE/TE/PO NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS

STEREO ATTRIBUTES: NONE

1582 SEA FILE=REGISTRY SSS FUL L3 L6 1038 SEA FILE=HCAPLUS ABB=ON L5 L7 17 SEA FILE=HCAPLUS ABB=ON L6(L)ELECTROLYT? 13 SEA FILE=HCAPLUS ABB=ON L7 AND ELECTROCHEM?/SC,SX,AB,BI L8 12 SEA FILE=HCAPLUS ABB=ON L6 AND BATTER? L9 14 CA references with whility L10 14\_SEA FILE=HCAPLUS ABB=ON L8 OR L9

=> d l10 bib abs ind hitstr 1-14

ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2005:368511 HCAPLUS

DN 142:433056

ΤI Secondary nonaqueous electrolyte battery

IN Koto, Tomoko

PA Japan Storage Battery Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

L10

DATE KIND APPLICATION NO. DATE ..... 20050428 JP 2003-348133 PΙ JP 2005116306 A2 20031007 2Q031007 PRAI JP 2003-348133 The battery has a cathode, containing a Li-Ni-Mn composite oxide :

Lix NiyMn2-y04- $\delta$  (0< x< 1.1; 0.45< yr< 0.55; and 0 $\leq$   $\delta$ < 0.4) as a cathode active mass, an anode, and a nonaq. electrolyte solution; where the electrolyte solution contains 0.1-20 mass%. phosphazene derivative

TC ICM H01M010-40

ICS H01M004-02; H01M004-58

52-2 (Electrochemical, Radiational, and Thermal Energy Technology)

ST secondary lithium battery cathode lithium manganese nickel oxide; battery electrolyte phosphazene deriv

IT Battery cathodes

Battery electrolytes

(cathodes containing lithium manganese nickel oxides and electrolytes containing phosphazene derivs. for secondary lithium batteries)

IT Polyphosphazenes

RL: MOA (Modifier or additive use); USES (Uses)

(cyclic; cathodes containing lithium manganese nickel oxides and electrolytes containing phosphazene derivs. for secondary lithium batteries)

Secondary batteries IT

> (lithium; cathodes containing lithium manganese nickel oxides and electrolytes containing phosphazene derivs. for secondary lithium batteries)

IT 96-48-0, γ-Butyrolactone 96-49-1, Ethylene carbonate 105-58-8, Diethyl carbonate 108-32-7, Propylene carbonate 616-38-6, Dimethyl carbonate 623-53-0, Ethyl methyl carbonate 7782-42-5, Graphite, uses 12031-75-3, Lithium manganese nickel oxide (LiMn1.5Ni0.504) 14283-07-9, Lithium tetrafluoroborate 21324-40-3, Lithium hexafluorophosphate RL: DEV (Device component use); USES (Uses)

(cathodes containing lithium manganese nickel oxides and electrolytes containing phosphazene derivs. for secondary lithium batteries)

850650-07-6 IT

RL: MOA (Modifier or additive use); USES (Uses) (cathodes containing lithium manganese nickel oxides and electrolytes containing phosphazene derivs. for secondary lithium batteries)

TТ 850650-07-6

> RL: MOA (Modifier or additive use); USES (Uses) (cathodes containing lithium manganese nickel oxides and electrolytes containing phosphazene derivs. for secondary lithium batteries)

RN 850650-07-6 HCAPLUS

Phosphoramidofluoridic acid, [difluoro[(trifluorophosphoranylidene)amino]p CN hosphoranylidene]-, ethyl ester (9CI) (CA INDEX NAME)

ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN T-10

AN 2004:589783 HCAPLUS

DN 141:126373

ΤI Separator for nonaqueous electrolyte battery

Kanno, Hiroshi; Otsuki, Masashi; Eguchi, Shinichi IN

PA Bridgestone Corporation, Japan

PCT Int. Appl., 32 pp. SO

CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE ----WO 2004062002 PT 20040722 WO 2003-JP16360 **A1** 20031219 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO,

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WEINER
         10/936148
                      08/10/2005
                                          RPage 4
             NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
             TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                20021227
PRAI JP 2002-380683
                          Α
     The separator, which is incombustible even when the inside of a
     battery has a high temperature and useful for a primary or secondary Li
     battery, comprises a micro-porous film formed by adding a
     phosphazene derivative and/or an isomer of a phosphazene derivative to a polymer.
IC
     ICM H01M002-16
     ICS H01M010-40
CC
     52-2 (Electrochemical, Radiational, and Thermal Energy Technology)
ST
     nonaq electrolyte battery incombustible separator phosphazene
     deriv added polymer
IT
     Primary battery separators
     Secondary battery separators
        (separators containing phosphazene derivative added polymers for primary and
        secondary lithium batteries)
IT
     7439-93-2, Lithium, uses
     RL: DEV (Device component use); USES (Uses)
        (anode; separators containing phosphazene derivative added polymers for primary
        and secondary lithium batteries)
IT
                                          12190-79-3, Cobalt lithium oxide
     1313-13-9, Manganese dioxide, uses
     (CoLiO2)
     RL: DEV (Device component use); USES (Uses)
        (cathode; separators containing phosphazene derivative added polymers for
        primary and secondary lithium batteries)
IT
     96-48-0, γ-Butyrolactone 96-49-1, Ethylene carbonate
     Diethyl carbonate 957-13-1
                                   1184-10-7 2397-48-0
                                                            9002-88-4,
     Polyethylene 14283-07-9, Lithium tetrafluoroborate
                                                            33027-68-8
     722454-84-4 722454-86-6
                               724792-59-0
     RL: DEV (Device component use); USES (Uses)
        (separators containing phosphazene derivative added polymers for primary and
        secondary lithium batteries)
IT
     724792-60-3
     RL: DEV (Device component use); USES (Uses)
        (separators containing phosphazene derivative added polymers for primary and
        secondary nonaq. electrolyte batteries)
IT
     722454-84-4 722454-86-6
    RL: DEV (Device component use); USES (Uses)
        (separators containing phosphazene derivative added polymers for primary and
        secondary lithium batteries)
RN
     722454-84-4 HCAPLUS
CN
     Phosphoramidic acid, (trifluorophosphoranylidene) -, diethyl ester (9CI)
     (CA INDEX NAME)
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RN 722454-86-6 HCAPLUS

CN Phosphorodifluoridimidic acid, acetyl-, phenyl ester (9CI) (CA INDEX NAME)

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WEINER
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PhO- P N- Ac
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ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
AN
     2004:570217 HCAPLUS
DN
     141:126304
TI
     Additive for secondary battery nonaqueous electrolyte solution
     and the battery
     Otsuki, Masashi; Horikawa, Yasuro
IN
PA
     Bridgestone Corporation, Japan
     PCT Int. Appl., 33 pp.
SO
     CODEN: PIXXD2
DТ
     Patent
LΑ
     Japanese
FAN.CNT 1
                                 DATE
     PATENT NO.
                          KIND
                                             APPLICATION NO.
                                                                      DATE
                                  (-/--\---
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                                              -----
                          ----
                                  20040715 WO 2003-JP16592
PΙ
     WO 2004059782
                           A1
                                                                      20031224
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO,
             NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
             TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRAI JP 2002-377142
                                 20021226
                          Α
     The additive comprises a phosphazene derivative represented by R13P = N-X (R1
     = halo or monovalent substituent; and X = C, Si, N, P, O and/or S containing
     organic group). The battery has a nonaq. electrolyte solution
     comprising the above additive, a cathode, and an anode.
IC
     ICM H01M010-40
     52-2 (Electrochemical, Radiational, and Thermal Energy
CC
     Technology)
     secondary lithium battery nonaq electrolyte additive phosphazene
ST
     deriv
IT
     Battery electrolytes
        (additives containing phosphazene derivs. for secondary battery
        electrolytes)
IT
     Secondary batteries
        (lithium; additives containing phosphazene derivs. for secondary
        battery electrolytes)
IT
     96-49-1, Ethylene carbonate
                                    105-58-8, Diethyl carbonate 12190-79-3,
     Cobalt lithium oxide (CoLiO2) 21324-40-3, Lithium hexafluorophosphate
     RL: DEV (Device component use); USES (Uses)
        (additives containing phosphazene derivs. for secondary battery
        electrolytes)
IT
     2397-48-0 722454-84-4
                              722454-85-5 722454-86-6
     RL: MOA (Modifier or additive use); USES (Uses)
        (additives containing phosphazene derivs. for secondary battery
        electrolytes)
IT
     722454-84-4 722454-86-6
```

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WEINER 10/936148 08/10/2005
```

RPage 6

RL: MOA (Modifier or additive use); USES (Uses) (additives containing phosphazene derivs. for secondary battery electrolytes)

RN 722454-84-4 HCAPLUS

CN Phosphoramidic acid, (trifluorophosphoranylidene)-, diethyl ester (9CI) (CA INDEX NAME)

RN 722454-86-6 HCAPLUS

CN Phosphorodifluoridimidic acid, acetyl-, phenyl ester (9CI) (CA INDEX NAME)

### RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:162949 HCAPLUS

DN 140:202437

TI Improvement of pigment-sensitized photoelectrochemical cell

IN Yoshikawa, Masato; Ohno, Shingo; Kobayashi, Taichi; Sugimura, Takayuki; Iwabuchi, Yoshinori; Shiino, Osamu; Sugiyama, Hideo; Horikawa, Yasuo; Toyosawa, Shinichi

PA Bridgestone Corporation, Japan

SO PCT Int. Appl., 110 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

FAN. CNT 1

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PATENT NO.
                          KIND
                                  DATE
                                              APPLICATION NO.
                                                                      DATE
                                              -----
                                  20040226
                                                                       20030806
ΡI
     WO 2004017452
                           A1
                                              WO 2003-JP9983
         W: AE, AG, AL, AM, AT, AT, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
             TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IFT IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                 2/0050601 EP 2003-788043
                           Α1
                                                                      20030806
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
PRAI JP 2002-235393
                                  20020813
                           Α
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(CA INDEX NAME)

#### RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:139816 HCAPLUS

140:184695 DN

Secondary nonaqueous electrolyte battery ΤI

Narioka, Yoshinori; Mori, Sumio IN

Japan Storage Battery Co., Ltd., Japan PA

Jpn. Kokai Tokkyo Koho, 14 pp. SO

CODEN: JKXXAF

DΤ Patent

Japanese LА

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
		- <i>//</i> -				
PI JP 2004055208	A2	20040219	JP 2002-208280	20020717		
PRAI JP 2002-208280		<del>2002</del> 0717				

AB

The battery has an active mass containing anode and a Li salt dissolved nonaq. electrolyte solution; where the electrolyte solution has a halo-containing phosphazene compound and the anode has a binder comprising a non-halo material.

ICM H01M010-40 IC

ICS H01M004-02; H01M004-62

52-2 (Electrochemical, Radiational, and Thermal Energy CC Technology)

ST secondary battery electrolyte halo contq phosphazene compd; anode binder nonhalo compd secondary battery

IT Fluoropolymers, uses

Styrene-butadiene rubber, uses

RL: DEV (Device component use); USES (Uses)

(anode binder; anode binders containing non-halo materials for secondary lithium batteries)

IT Battery anodes

(anode binders containing non-halo materials for secondary lithium batteries)

IT Battery electrolytes

> (electrolyte solns. having halo-containing phosphazene compds. for secondary lithium batteries)

IT Secondary batteries

> (secondary lithium batteries having halo-containing phosphazene compds. in electrolyte solns. and non-halo materials in anodes)

ΙT 7782-42-5, Graphite, uses

RL: DEV (Device component use); USES (Uses)

(anode active mass; anode binders containing non-halo materials for secondary lithium batteries)

IT 24937-79-9, Pvdf

RL: DEV (Device component use); USES (Uses)

(anode binder; anode binders containing non-halo materials for secondary lithium batteries)

96-49-1, Ethylene carbonate 105-58-8, Diethyl carbonate IT Lithium hexafluorophosphate 657348-91-9

ior se

RL: DEV (Device component use); USES (Uses) (electrolyte solns. having halo-containing phosphazene compds.

for secondary lithium batteries)

IT 9003-55-8

RL: DEV (Device component use); USES (Uses)

(styrene-butadiene rubber, anode binder; anode binders containing non-halo materials for secondary lithium **batteries**)

IT 657348-91-9

RL: DEV (Device component use); USES (Uses)

(electrolyte solns. having halo-containing phosphazene compds.

for secondary lithium batteries)

RN 657348-91-9 HCAPLUS

CN Phosphinimidic fluoride, N-ethoxy-P,P-bis(pentafluoroethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:396161 HCAPLUS

DN 138:392003

TI Low-temperature electrolysis of alkali metal halides for metal preparation

IN Jacobson, Stephen Ernest; Mah, Dennie Turin

PA USA

SO U.S. Pat. Appl. Publ., 8 pp.

CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1 APPLICATION NO. KIND DATE PATENT NO. \_\_\_\_ \_\_\_\_\_\_ ------20030522 US 2001-989880 ΡI US 2003094379 **A**1 20040907 US 6787019 B2 PRAI US 2001-989880 20011121

AB A low temperature electrolysis process that can be used for producing an alkali metal from an alkali metal halide is provided, which comprises electrolyzing an electrolyte composition comprising at least one alkali metal halide and a co-electrolyte comprising (a) a halide or halides of Group IIIA, Group IB, or Group VIII metals and (b) a halide-donating compound

IC ICM C21B015-00

INCL 205406000; 075711000

CC 72-5 (Electrochemistry)

Section cross-reference(s): 49, 56

ST low temp electrolysis alkali metal halides halide donation compd; alkali metal prep electrolysis low temp halide

IT Alkali metal halides, reactions

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(low-temperature electrolysis for metal preparation)

IT Electrolysis

(low-temperature electrolysis of alkali metal halides for metal preparation)

IT Salts, uses

RL: NUU (Other use, unclassified); USES (Uses)

(molten; low-temperature electrolysis of alkali metal halides for metal

preparation in electrolyte containing halide donation compound)

IT Halides

RL: NUU (Other use, unclassified); PNU (Preparation, unclassified); PREP (Preparation); USES (Uses)

(of aluminum, boron, nickel, antimony, iron, cobalt; low-temperature electrolysis of alkali metal halides for metal preparation in electrolyte containing)

IT Alkali metals, processes

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PREP (Preparation); PROC (Process)

(preparation by low-temperature electrolysis of alkali metal halides)

IT 7782-50-5, Chlorine, processes

RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); FORM (Formation, nonpreparative); PROC (Process)

(formation during low-temperature electrolysis of alkali metal halides for metal preparation in electrolyte containing halide donation compound)

IT 7647-14-5, Sodium chloride, reactions

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(low-temperature electrolysis for metal preparation in electrolyte containing AlCl3 and trichlorophosphazosulfonyl chloride)

IT 124-63-0, Methanesulfonyl chloride 14700-21-1,

Trichlorophosphazosulfonyl chloride

RL: NUU (Other use, unclassified); USES (Uses)

(low-temperature electrolysis of alkali metal halides for metal preparation in **electrolyte** containing)

IT 7446-70-0P, Aluminum chloride, uses 13966-08-0P

RL: NUU (Other use, unclassified); PNU (Preparation, unclassified); PREP (Preparation); USES (Uses)

(low-temperature electrolysis of alkali metal halides for metal preparation in electrolyte containing)

IT 7440-23-5P, Sodium, processes

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PREP (Preparation); PROC (Process)

(preparation by low-temperature electrolysis of sodium chloride in electrolyte containing AlCl3 and trichlorophosphazosulfonyl chloride)

IT 14700-21-1, Trichlorophosphazosulfonyl chloride

RL: NUU (Other use, unclassified); USES (Uses)

(low-temperature electrolysis of alkali metal halides for metal preparation in **electrolyte** containing)

RN 14700-21-1 HCAPLUS

CN Sulfamoyl chloride, (trichlorophosphoranylidene) - (7CI, 8CI, 9CI) (CA INDEX NAME)

$$\begin{array}{c}
0 \\
|| \\
|| \\
0
\end{array}$$

IT 13966-08-0P

RL: NUU (Other use, unclassified); PNU (Preparation, unclassified); PREP (Preparation); USES (Uses)

(low-temperature electrolysis of alkali metal halides for metal preparation in electrolyte containing)

RN 13966-08-0 HCAPLUS

CN Phosphorimidic trichloride, (dichlorophosphinyl) - (6CI, 8CI, 9CI) (CA INDEX NAME)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:873246 HCAPLUS

136:20156 DN

ТT Preparation of sulfonyl-containing phosphazenes

Narita, Yukio; Saito, Tadashi; Ohara, Nobuhiko; Wakui, Atsushi; Kamata, TN

PA Nippon Chemical Industrial Co., Ltd., Japan

Jpn. Kokai Tokkyo Koho, 7 pp. SO CODEN: JKXXAF

DТ Patent

Japanese LA

FAN.CNT 1

I	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 2001335590 JP 2000-157053	A2	2001 <sup>1</sup> 1204 2000 <sup>0</sup> 526	JP 2000-157053	20000526

os CASREACT 136:20156; MARPAT 136:20156

The title (R10)3P:NSO2R2 [R1 = (CH2CH2O)nMe which may be substituted with AB halo (n = 1-5); R2 = C1-12 (halo) alkyl, (halo) phenyl, C1-4 alkyl-(halo)phenyl] (I), useful as electrolytes for nonag. secondary batteries, flame retardants for lubricants, etc., are prepared by treating phosphorus pentahalides with H2NSO2R2 (R2 = same as above) and then treating the resulting X3P:NSO2R2 (R2 = same as above; X = halo) (II) with R1OM (R1 = same as above; M = alkali metal). E.g., a mixture of PCl5, PhSO2NH2, toluene, and THF was stirred at room temperature for 2.5 h to give 96.9% II (R2 = Ph, X = Cl) (III). An alcoholate solution, prepared from MeOCH2CH2OH and NaH in THF, was added dropwise to a mixture of III and toluene at 0-10° and then the reaction mixture was stirred at room temperature for 3.5 h to give 78.4% I (R1 = CH2CH2OMe, R2 = Ph).

IC ICM C07F009-24

ICS H01G009-038; H01G009-035; H01M006-16; H01M010-40

CC 29-7 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 52

ST methoxyethylphosphazosulfonylbenzene prepn electrolyte nonag secondary battery; phosphazosulfonyl compd prepn electrolyte nonag secondary battery; phosphorus pentahalide condensation sulfonamide; halophosphazosulfonyl compd condensation glycol ether alcoholate

IT Battery electrolytes

(preparation of phosphazosulfonyl compds. as electrolytes for nonaq. secondary batteries)

IT Phosphazenes

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of phosphazosulfonyl compds. as electrolytes for nonag. secondary batteries)

IT 111-77-3P, Diethylene glycol monomethyl ether 1525-81-1P,
 N-4-Fluorobenzenesulfonyl-P,P,P-trichlorophosphazene 5666-55-7P,
 Trichlorophosphazosulfonylbenzene 19278-10-5P, Diethylene glycol
 monomethyl ether sodium salt 29651-24-9P 377780-52-4P,
 N-2,4-Difluorobenzenesulfonyl-P,P,P-trichlorophosphazene
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
 preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of phosphazosulfonyl compds. as electrolytes for
 nonaq. secondary batteries)

IT 377780-53-5P 377780-54-6P 377780-55-7P 377780-56-8P RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of phosphazosulfonyl compds. as electrolytes for nonaq. secondary batteries)

IT 98-10-2, Benzenesulfonamide 109-86-4, Ethylene glycol monomethyl ether 402-46-0, 4-Fluorobenzenesulfonamide 3139-99-9, Ethylene glycol monomethyl ether sodium salt 3144-09-0, Methanesulfonamide 10026-13-8, Phosphorus pentachloride 13656-60-5, 2,4-Difluorobenzenesulfonamide RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of phosphazosulfonyl compds. as electrolytes for nonaq. secondary batteries)

IT 1525-81-1P, N-4-Fluorobenzenesulfonyl-P,P,P-trichlorophosphazene
5666-55-7P, Trichlorophosphazosulfonylbenzene 29651-24-9P
377780-52-4P, N-2,4-Difluorobenzenesulfonyl-P,P,Ptrichlorophosphazene
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of phosphazosulfonyl compds. as electrolytes for
 nonaq. secondary batteries)

RN 1525-81-1 HCAPLUS

CN Phosphorimidic trichloride, [(4-fluorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 5666-55-7 HCAPLUS

CN Phosphorimidic trichloride, (phenylsulfonyl) - (6CI, 8CI, 9CI) (CA INDEX NAME)

$$\begin{array}{c} \overset{O}{\parallel} \\ \text{ph-} \overset{O}{\parallel} \\ \overset{\parallel}{\parallel} \\ \overset{O}{\longrightarrow} \end{array} \text{PCl}_{3}$$

CN

RN 29651-24-9 HCAPLUS

Phosphorimidic trichloride, (methylsulfonyl) - (8CI, 9CI) (CA INDEX NAME)

WEINER

RN 377780-52-4 HCAPLUS

CN Phosphorimidic trichloride, [(2,4-difluorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

L10 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:369718 HCAPLUS

DN 134:367047

TI Preparation of sulfonyl-containing phosphazenes as flame retardants for battery electrolytes

IN Tsuchiya, Tsubasa; Kawakabe, Hiroshi; Wakui, Atsushi; Kamata, Tomohisa

PA Nippon Chemical Industrial Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 2001139584	A2	2001 0522	JP 1999-325440	19991116
PRAI JP 1999-325440		199 <b>9</b> 1116		

OS CASREACT 134:367047; MARPAT 134:367047

AB Title compds. (R10)3P:NSO3R1 or (R20)3P:NSO2N:P(OR2)3 [R1, R2 = (ether-containing) C1-10 alkyl, haloalkyl] are prepared by reaction of PX5 (X = halo) with sulfamic acid or sulfamide followed by ROM (R = same as R1 or R2; M = alkali metal). PCl5 was treated with sulfamic acid in PhCl at 100-105° for 12 h to give 68.8% Cl3P:NSO2Cl, which was treated with diethylene glycol monomethyl ether alcoholate in THF at -22 to -20° for 1 day to give 75.2% (MeOC2H4OC2H4O)3P:NSO3C2H4OC2H4OMe.

IC ICM C07F009-24 ICS C09K021-12

CC 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 52

sulfonyl phosphazene prepn flame retardant electrolyte; battery electrolyte flame retardant phosphazene prepn; sulfamic acid reaction phosphorus pentahalide alcoholate; sulfamide reaction phosphorus pentahalide alcoholate

IT Battery electrolytes

Fireproofing agents

(preparation of sulfonyl-containing phosphazenes as flame retardants for battery electrolytes)

IT Metal alkoxides

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of sulfonyl-containing phosphazenes as flame retardants for battery electrolytes)

IT 109-86-4D, Ethylene glycol monomethyl ether, salts 111-77-3D, Diethylene glycol monomethyl ether, salts 141-52-6, Sodium ethoxide 5329-14-6, Sulfamic acid 7803-58-9, Sulfamide 10026-13-8, Phosphorus pentachloride

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of sulfonyl-containing phosphazenes as flame retardants for battery electrolytes)

IT 14259-65-5P, Bis(trichlorophosphazo) sulfone 14700-21-1P

Trichlorophosphazosulfonyl chloride

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of sulfonyl-containing phosphazenes as flame retardants for battery electrolytes)

IT 72250-12-5P 271771-13-2P 271771-14-3P 271771-15-4P

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of sulfonyl-containing phosphazenes as flame retardants for battery electrolytes)

IT 14259-65-5P, Bis(trichlorophosphazo) sulfone 14700-21-1P

, Trichlorophosphazosulfonyl chloride

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of sulfonyl-containing phosphazenes as flame retardants for battery electrolytes)

RN 14259-65-5 HCAPLUS

CN Phosphorimidic trichloride, sulfonylbis- (9CI) (CA INDEX NAME)

$$\begin{array}{c}
\text{Cl}_{3}\text{P} = \text{N} - \text{S} - \text{N} = \text{PCl}_{3} \\
\parallel \\
\text{O}
\end{array}$$

RN 14700-21-1 HCAPLUS

CN Sulfamoyl chloride, (trichlorophosphoranylidene) - (7CI, 8CI, 9CI) (CA INDEX NAME)

L10 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1998:686074 HCAPLUS

DN 130:25419

TI Polyphosphazenes with Novel Architectures: Influence on Physical Properties and Behavior as Solid Polymer Electrolytes

AU Allcock, Harry R.; Sunderland, Nicolas J.; Ravikiran, Ramakrishna; Nelson, James M.

CS Department of Chemistry, The Pennsylvania State University, University Park, PA, 16802, USA

SO Macromolecules (1998), 31(23), 8026-8035

CODEN: MAMOBX; ISSN: 0024-9297
PB American Chemical Society

DT Journal LA English

AB Three types of polyphosphazenes with different architectures have been synthesized and characterized. The influence of the polymer architecture on solid ionic conductivity was of particular interest. The first type includes linear oligo- and polyphosphazenes with the general formula [N:P(OCH2CH2OCH2CH2OCH3)2]n (MEEP) with different chain lengths. second type consists of a series of tri-armed star-branched polyphosphazenes with the general formula N{CH2CH2NH(CF3CH2O)2P[N:P(OCH2CH 20CH2CH2OCH3)2]n}3 with different arm lengths. These were synthesized via the reaction of the tridentate initiator [N{CH2CH2NH(CF3CH2O)2P:N-PC13+}3] [PC16-]3 with the phosphoranimine Cl3P:NSiMe3 in CH2Cl2 followed by halogen replacement with sodium (methoxyethoxy) ethoxide. The mol. wts. in this system were carefully controlled by variation of the monomer-to-initiator ratios, and the effect of polymer mol. weight on solid ionic conductivity was examined The third polymer system was designed to examine the effect of complex branching on ionic conductivity Thus, a highly branched polymer containing five branches from a cyclotriphosphazene pendent side group (with 26 ethyleneoxy units per repeat unit) was synthesized. The conductivity of this polymer in the presence of three different salts has been measured and compared to the behavior of MEEP with a corresponding mol. weight The mechanism of ion transport in these systems is discussed.

CC 35-7 (Chemistry of Synthetic High Polymers) Section cross-reference(s): 37, 52, 76

ST polyphosphazene novel structure lithium complex ionic cond

IT Polymerization

Polymerization

Polymerization catalysts

Polymerization catalysts

(cationic, living; preparation of polyphosphazenes with novel architecture, their phys. properties, and ionic conductivity of solid polymer electrolytes prepared by complexation of polyphosphazenes with lithium)

IT Battery electrolytes

Glass transition temperature

Ionic conductivity

Molecular weight

Polymer electrolytes

(preparation of polyphosphazenes with novel architecture, their phys. properties, and ionic conductivity of solid polymer electrolytes prepared by complexation of polyphosphazenes with lithium)

IT 131841-09-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(byproduct in preparation of polyphosphazenes with novel architecture, their phys. properties, and ionic conductivity of solid polymer electrolytes prepared by complexation of polyphosphazenes with lithium)

IT 10026-13-8, Phosphorus pentachloride

RL: CAT (Catalyst use); USES (Uses)

(catalyst; preparation of polyphosphazenes with novel architecture, their phys. properties, and ionic conductivity of solid polymer electrolytes prepared by complexation of polyphosphazenes with lithium)

IT 33454-82-9, Lithium triflate

RL: MOA (Modifier or additive use); USES (Uses)

(electrolytes; preparation of polyphosphazenes with novel architecture, their phys. properties, and ionic conductivity of solid polymer electrolytes prepared by complexation of polyphosphazenes with lithium)

IT 188186-00-7 216530-14-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(initiator used as core for branched polyphosphazenes; preparation of

polyphosphazenes with novel architecture, their phys. properties, and ionic conductivity of solid polymer electrolytes prepared by complexation of polyphosphazenes with lithium)

- 1T 19278-10-5DP, 2-(2-Methoxyethoxy)ethanol sodium salt, reaction products
  with poly(dichlorophosphazene), lithium complexes 26085-02-9DP,
  Poly(dichlorophosphazene), derivs., lithium complexes 40678-60-2DP
  , derivs., lithium complexes
  - RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (linear and branched; preparation of polyphosphazenes with novel architecture, their phys. properties, and ionic conductivity of solid polymer electrolytes prepared by complexation of polyphosphazenes with lithium)
- IT 216530-18-6DP, reaction products with poly(dichlorophosphazene), lithium complexes
  - RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation of polyphosphazenes with novel architecture, their phys. properties, and ionic conductivity of solid polymer electrolytes prepared by complexation of polyphosphazenes with lithium)
- TT 7439-93-2DP, Lithium, complexes with polyphosphazenes, preparation
  RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
  (Reactant or reagent)

(preparation of polyphosphazenes with novel architecture, their phys. properties, and ionic conductivity of solid polymer electrolytes prepared by complexation of polyphosphazenes with lithium)

IT 110-87-2 112-27-6 19278-10-5, 2-(2-Methoxyethoxy) ethanol sodium salt RL: RCT (Reactant); RACT (Reactant or reagent) (reactant in preparation of polyphosphazenes with novel architecture, their phys. properties, and ionic conductivity of solid polymer electrolytes prepared by complexation of polyphosphazenes with lithium)

IT 60221-37-6P 132939-00-5P 216530-17-5P 216530-18-6P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparat

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

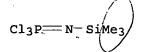
(reactant in preparation of polyphosphazenes with novel architecture, their phys. properties, and ionic conductivity of solid polymer electrolytes prepared by complexation of polyphosphazenes with lithium)

IT 40678-60-2DP, derivs., lithium complexes

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (linear and branched; preparation of polyphosphazenes with novel architecture, their phys. properties, and ionic conductivity of solid polymer electrolytes prepared by complexation of polyphosphazenes with lithium)

RN 40678-60-2 HCAPLUS

CN Phosphorimidic trichloride, (trimethylsilyl) - (9CI) (CA INDEX NAME)



RE.CNT 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1998:681962 HCAPLUS

DN 129:262843

- TI High conductivity electrolyte solutions and secondary batteries using the solutions
- IN Angell, Charles Austen; Zhang, Sheng-Shui; Xu, Kang
- PA Arizona Board of Regents, USA
- SO U.S., 14 pp. CODEN: USXXAM

DT Patent LA English FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE ---------US 5824433 Α 19981020 US 1996-748009 19961112 PΤ PRAI US 1996-748009 19961112 MARPAT 129:262843 os The electrolyte solns. contain an electrolyte solute and a AB sulfonyl/phospho compound solvent RSO2X (X = halide and R = perfluoroalkyl group, perchlorinated group, N:PX3) or X3P:NR' [R' = P(O)X2 or C1-6 alkyl group]. The solvent may contain Cl3PNSO2Cl, Cl3PNP(O)Cl2, Cl3PNCH3, CL3PNCH2CH3, and/or CF3(CF2)3SO2F; and the electrolyte solute os LiAlCl4 or (CF3SO2)2NLi. The electrolyte may also contain a polymer. ICM H01M006-14 INCL 429194000 52-2 (Electrochemical, Radiational, and Thermal Energy CC Technology) ST lithium battery electrolyte solvent; battery electrolyte solvent sulfur phosphorous compd IT Battery electrolytes (high conductivity electrolyte solns. containing sulfur-phosphorus compound electrolyte solvents for secondary lithium batteries and sodium/sulfur batteries) IT 124-63-0, Methanesulfonyl chloride 9011-14-7, Pmma 14024-11-4, Aluminum lithium chloride (LiAlCl4) 90076-65-6 RL: DEV (Device component use); USES (Uses) (high conductivity electrolyte solns. containing sulfur-phosphorus compound electrolyte solvents for secondary batteries) IT 13966-08-0P 14700-21-1P 23453-30-7P 44584-14-7P RL: DEV (Device component use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses) (high conductivity electrolyte solns. containing sulfur-phosphorus compound electrolyte solvents for secondary batteries 13966-08-0P 14700-21-1P 23453-30-7P TΤ 44584-14-7P RL: DEV (Device component use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses) (high conductivity electrolyte solns. containing sulfur-phosphorus compound electrolyte solvents for secondary batteries 13966-08-0 HCAPLUS RNPhosphorimidic trichloride, (dichlorophosphinyl) - (6CI, 8CI, 9CI) (CA CN INDEX NAME)

14700-21-1 HCAPLUS RN

CN Sulfamoyl chloride, (trichlorophosphoranylidene) - (7CI, 8CI, 9CI) (CA INDEX NAME)

WEINER

RN 23453-30-7 HCAPLUS

CN Phosphorimidic trichloride, methyl- (8CI, 9CI) (CA INDEX NAME)

 $Cl_3P == N-Me$ 

RN 44584-14-7 HCAPLUS

CN Phosphorimidic trichloride, ethyl- (9CI) (CA INDEX NAME)

C13P --- N- Et

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

Lio ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1997:443306 HCAPLUS

DN 127:53454

TI **Electrochemically** stable electrolytes which do not crystallize at ambient temperature

IN Angell, Charles Austen; Zhang, Sheng Shui; Xu, Kang

PA Arizona Board of Regents, USA

SO PCT Int. Appl., 31 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PAN.	CNI	Т																		
	PATENT NO.					KIN	KIND DATE			APPLICATION NO.							DATE			
							-								<del>-</del>	-				
ΡI	WO	9718	159			A1		19970522		WO 1996-US18325						19961113				
		W:	AL,	AM,	AT,	ΑU,	AZ,	BB,	ВG,	BR,	BY,	CA,	CH,	CN,	CZ,	DE,	DK,	EE,		
			ES,	FI,	GB,	GE,	HU,	IL,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	KZ,	LK,	LR,	LS,		
			LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,		
			SE,	SG,	SI,	SK,	TJ,	TM,	TR,	TT,	UA,	UG,	UΖ,	VN,	AM,	ΑZ,	BY,	KG,		
			ΚZ,	MD,	RU,	ТJ,	TM													
		RW:	KΕ,	LS,	MW,	SD,	SZ,	ŪĠ,	ΑT,	ΒE,	CH,	DE,	DK,	ES,	FI,	FR,	GB,	GR,		
			ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	ML,		
	·		MR,	ΝE,	SN,	TD,	TG													
	US	5855	809			A		1999	0105	US 1996-748008						19961112				
	ΑU	9676	807			A1		1997	0605		AU 1:	996-	7680	7		19961113				
PRAI	US	1995	-643	7P		P		1995	1113	}										
	US	1996	-748	800		Α		1996	1112											
•	WO	1996	-US1	8325		W		1996	1113											
7 77	ml.	1-		3 t								_ 7.2			i					

AB The electrolytes are quasi-salt inorg. ionic liqs. which comprise the reaction product of a strong Lewis acid with an inorg. halide-donating mol., which comprises a substructure selected from NPX3, SO2X, and C(O)X, where X is a halogen. The strong Lewis acid is selected from AlCl3, BCl3, SbCl3, and FeCl3. These quasi-salt inorg. ionic liquid mixts. are useful electrolytes.

IC ICM C01B021-06

ICS C01B025-10; C01C001-02; H01B001-00

WEINER 10/936148 08/10/2005 RPage 19 CC 52-2 (Electrochemical, Radiational, and Thermal Energy Technology) Section cross-reference(s): 49 ST battery electrolyte electrochem stable; halide donating mol Lewis acid electrolyte IT Battery electrolytes (electrochem. stable which do not crystallize at ambient temperature) IT 7446-70-0D, Aluminum chloride (AlCl3), reaction product with inorg. halide-donating mol., processes 7705-08-0D, Iron chloride (FeCl3), reaction product with inorg. halide-donating mol., processes 10025-91-9D, Antimony chloride (SbCl3), reaction product with inorg. halide-donating mol. 10294-34-5D, Boron chloride (BCl3), reaction product with inorg. halide-donating mol. RL: PEP (Physical, engineering or chemical process); PROC (Process)

(electrochem. stable electrolytes from)

75-36-5DP, Acetyl chloride, reaction product with aluminum chloride

13966-08-0DP, reaction product with aluminum chloride

14700-21-1DP, reaction product with aluminum chloride

23453-30-7DP, reaction product with aluminum chloride

44584-14-7DP, reaction product with boron chloride

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process) (electrochem. stable electrolytes from)

2926-30-9, Sodium trifluoromethanesulfonate 7784-16-9, Sodium chloroaluminate 14024-11-4, Lithium chloroaluminate 33454-82-9, Lithium trifluoromethanesulfonate 90076-65-6, Lithium bis(trifluoromethylsulfonyl)imide 91742-21-1, Sodium bis(trifluoromethylsulfonyl)imide

RL: MOA (Modifier or additive use); USES (Uses)

(quasi-salt inorg. ionic liquid electrolytes containing)

13966-08-0DP, reaction product with aluminum chloride 14700-21-1DP, reaction product with aluminum chloride 23453-30-7DP, reaction product with aluminum chloride 44584-14-7DP, reaction product with boron chloride

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(electrochem. stable electrolytes from)

RN 13966-08-0 HCAPLUS

IT

IT

RN 14700-21-1 HCAPLUS

CN Sulfamoyl chloride, (trichlorophosphoranylidene) - (7CI, 8CI, 9CI) (CA INDEX NAME)

RN23453-30-7 HCAPLUS

CN Phosphorimidic trichloride, methyl- (8CI, 9CI) (CA INDEX NAME)

 $Cl_3P = N-Me$ 

RN 44584-14-7 HCAPLUS

CN Phosphorimidic trichloride, ethyl- (9CI) (CA INDEX NAME)

 $Cl_3P = N - Et$ 

L10 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1997:440216 HCAPLUS

DN 127:53456

Sulfonyl/phospho-compound solvent for high-conductivity electrolyte ΤI solutions and secondary batteries incorporating these solutions

IN Angell, Charles Austen; Zhang, Sheng Shui; Xu, Kang

PA Arizona State University, Board of Regents, USA

SO PCT Int. Appl., 21 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

		_															,				
	PATENT NO.				KIND DATE			1	APPL	ICAT	DATE										
							-														
PI	WO	9718	595			A1	A1 19970522		0522	WO 1996-US18324						19961113					
		W:	AL,	AM,	AT,	AU,	ΑZ,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CZ,	DE,	DK,	EE,			
			ES,	FI,	GB,	GE,	HU,	IL,	ıs,	JP,	ΚE,	KG,	KΡ,	KR,	ΚZ,	LK,	LR,	LS,			
			LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	ΝŻ,	PL,	PT,	RO,	RU,	SD,			
			SE,	SG,	SI,	SK,	ТJ,	TM,	TR,	TT,	UA,	UG,	UΖ,	VN,	AM,	ΑZ,	BY,	KG,			
			ΚZ,	MD,	RU,	TJ,	TM														
		RW:	KΕ,	LS,	MW,	SD,	SZ,	ŪĠ,	ΑT,	ВE,	CH,	DE,	DK,	ES,	FI,	FR,	GB,	GR,			
			ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	ML,			
			MR,	NE,	SN,	TD,	TG														
	ΑU	9710	524			A1		1997	0605	AU 1997-10524						1:	9961	113			
PRAI	US	1995	-643	SP		P		1995	1113												
	WO	1996	-US1	3324		W		1996	1113												
os	MARPAT 127:53456																				

AB The solvent is selected from Cl3PNSO2Cl, Cl3PNP(O)Cl2, Cl3PNCH3, and Cl3PNCH2CH3. A sulfonyl/phospho-compound electrolyte solution comprises an electrolyte solute and a sulfonyl/phospho-compound electrolyte solvent.

IC ICM H01M006-14

ICS H01M006-16; H01M006-04

CC 52-2 (Electrochemical, Radiational, and Thermal Energy Technology)

Section cross-reference(s): 49, 76

ST battery electrolyte solvent sulfonyl phospho compd

IT Battery electrolytes WEINER 10/936148 08/10/2005

RPage 21

(sulfonyl/phospho-compound solvent for high-conductivity)

IT 124-63-0, Methyl sulfonyl chloride

RL: DEV (Device component use); USES (Uses)

(solvent for high-conductivity battery electrolyte solns.)

IT 13966-08-0P 14700-21-1P 23453-30-7P

44584-14-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(solvent for high-conductivity battery electrolyte solns.)

IT 13966-08-0P 14700-21-1P 23453-30-7P

44584-14-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(solvent for high-conductivity battery electrolyte solns.)

RN 13966-08-0 HCAPLUS

RN 14700-21-1 HCAPLUS

CN Sulfamoyl chloride, (trichlorophosphoranylidene) - (7CI, 8CI, 9CI) (CA INDEX NAME)

$$\begin{array}{c}
O \\
|| \\
S - N = PCl_3
\end{array}$$

RN 23453-30-7 HCAPLUS

CN Phosphorimidic trichloride, methyl- (8CI, 9CI) (CA INDEX NAME)

 $Cl_3P = N-Me$ 

RN 44584-14-7 HCAPLUS

CN Phosphorimidic trichloride, ethyl- (9CI) (CA INDEX NAME)

 $Cl_3P = N - Et$ 

L10 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1996:744515 HCAPLUS

DN 126:149660

TI Room temperature inorganic "quasi-molten salts" as alkali-metal electrolytes

AU Xu, K.; Zhang, S.; Angell, C. A.

CS Dep. Chem., Arizona State Univ., Tempe, AZ, 85287-1604, USA

SO Journal of the Electrochemical Society (1996), 143(11), 3548-3554 CODEN: JESOAN; ISSN: 0013-4651

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10/936148
                      08/10/2005
WEINER
                                          RPage 22
PB
     Electrochemical Society
DT
     Journal
LΑ
     English
AB
     Room temperature inorg. liqs. of high ionic conductivity were prepared by reacting
Lewis
     acid AlCl3 with sulfonyl chlorides. The mechanism is not clear at this
     time since a crystal structure study of the 1:1 complex with CH3SO2Cl (Tm
     = 30°) is not consistent with a simple chloride transfer to create
     AlClO4- anions. The liquid is in a state somewhere between ionic and mol.
     A new term quasi-molten salt is adopted to describe this state. A
     comparably conducting liquid can be made using BC13 in place of AlC13.
     Unlike their organic counterparts based on ammonium cations (e.g., pyridinium
     or imidazolium) which reduce in the presence of alkali metals, this inorg.
     class of cation shows great stability against electrochem. reduction
     (.apprx.-1.0 V vs. Li+/Li), with the useful consequence that reversible
     lithium and sodium metal deposition/stripping can be supported. The
     electrochem. window for these quasi-salts with AlCl3 ranges up to
     5.0 V, and their room temperature conductivities exceed 10-4 S/cm.
     dissolve lithium and sodium tetrachloroaluminates up to mole fraction
     .apprx.0.6 at 100° and intermediate compns. are permanently stable
     at ambient. The resultant lithium or sodium salt solns. exhibit
     electrochem. windows of 4.5-5.0 V vs. Li+/Li or Na+/Na and show
     room temperature conductivities of 10-30 .apprx. 10-25 S/cm. In preliminary
     charge/discharge tests, the cell Li/quasi-ionic liquid
     electrolyte/Li1+xMn2O4 showed a discharge capacity of .apprx.110 mA-h/(g
     of cathode) and sustained 80% of the initial capacity after 60 cycles,
     indicating that these quasi-molten salt-based electrolytes are promising
     candidates for alkali-metal batteries.
CC
     72-2 (Electrochemistry)
     Section cross-reference(s): 52, 68, 76
ST
     room temp inorg quasi molten salt; alkali metal electrolyte quasi molten
     salt; sulfonyl aluminum chloride melt electrochem window;
    phosphoryl aluminum chloride melt electrochem window;
     electrochem potential window sulfonyl phosphoryl chloroaluminate;
    battery electrolyte inorg quasi molten salt
IT
    Electric potential
        (electrochem. potential window of room temperature inorg.
        quasi-molten salts from aluminum chloride and sulfonyl chloride or
       phosphoryl chloride)
IT
    Battery electrolytes
        (of sulfonyl chloride or phosphoryl chloride compds. with aluminum
        chloride)
IT
     Ionic conductivity
        (of sulfonyl chloride or phosphoryl chloride compds. with aluminum
        chloride or boron chloride)
    7784-16-9, Sodium tetrachloroaluminate
IT
    RL: PEP (Physical, engineering or chemical process); PRP (Properties);
    PROC (Process)
        (cyclic voltammetry of NaAlCl4 in trichlorophosphazosulfonyl
```

chloride-aluminum chloride compound)
IT 14024-11-4, Lithium tetrachloroaluminate

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(cyclic voltammetry of trichlorophosphazosulfonyl chloride-aluminum chloride compound with and without LiAlCl4 and of LiAlCl4 in methanesulfonyl chloride)

IT 186696-36-6P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(electrochem. potential window and room temperature inorg.

METHER 10/33014

quasi-molten salts as alkali-metal electrolytes)

IT 186696-38-8P 186696-40-2P 186696-41-3P 186696-43-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (ionic conductivity and **electrochem.** potential window and room temperature inorg. quasi-molten salts as alkali-metal electrolytes)

IT 75-23-0, Ethylamine-boron trifluoride complex (1:1) 593-51-1, Methylamine hydrochloride 5329-14-6, Sulfamic acid 7783-20-2,

Diammonium sulfate, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction with PCl5)

(reaction with PC15)

IT 75-36-5, Acetyl chloride 124-63-0, Methanesulfonyl chloride
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)

(reaction with aluminum chloride: electrochem. potential window and room temperature inorg. quasi-molten salts as alkali-metal electrolytes)

IT 6041-61-8P 13966-08-0P 14700-21-1P,

Trichlorophosphazosulfonyl chloride

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(reaction with aluminum chloride: electrochem. potential

window and room temperature inorg. quasi-molten salts as alkali-metal electrolytes)

IT 7446-70-0, Aluminum chloride, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with sulfonyl chloride or phosphoryl chloride for quasi-molten salts)

IT 13966-08-0P 14700-21-1P, Trichlorophosphazosulfonyl

chloride

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(reaction with aluminum chloride: electrochem. potential

window and room temperature inorg. quasi-molten salts as alkali-metal
electrolytes)

RN 13966-08-0 HCAPLUS

CN Phosphorimidic trichloride, (dichlorophosphinyl) - (6CI, 8CI, 9CI) (CA INDEX NAME)

RN 14700-21-1 HCAPLUS

CN Sulfamoyl chloride, (trichlorophosphoranylidene) - (7CI, 8CI, 9CI) (CA INDEX NAME)

L10 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN AN 1996:582562 HCAPLUS

DN 125:252809

TI Inorganic electrolyte solutions and gels for rechargeable lithium batteries

AU Xu, Kang; Day, Natalie D.; Angell, C. Austen

CS Dep. Chem., Arizona State Univ., Tempe, AZ, 85287-1604, USA

SO Journal of the Electrochemical Society (1996), 143(9), L209-L211 CODEN: JESOAN; ISSN: 0013-4651

PB Electrochemical Society

DT Journal

LA English

AB A class of inorg. oxychloride compds. have been evaluated for use as electrolytic solvents in rechargeable lithium batteries.

Compared with SO2-based electrolytes, these showed much improved safety while maintaining room temperature conductivities of 10-3-10-2 S/cm and electrochem. voltage windows of 4.5-5.5 V vs. Li+/Li and supporting reversible Li metal deposition/stripping. With the addition of 2-5% polymer, the solns. acquire rubbery character with little loss of conductivity and no change in electrochem. stability. Preliminary charge/discharge tests with intercalation-type cathode as well as sulfur-based cathode showed that these inorg. electrolytes can operate with excellent reversibility.

CC 52-2 (Electrochemical, Radiational, and Thermal Energy Technology)

ST lithium battery inorg electrolyte soln gel; safety lithium battery inorg electrolyte oxychloride

IT Battery electrolytes

(inorg. electrolyte solns. and gels for rechargeable lithium batteries)

IT Electric conductivity and conduction

(ionic, inorg. electrolyte solns. and gels for rechargeable lithium batteries)

IT 9011-14-7, Pmma

RL: MOA (Modifier or additive use); USES (Uses) (electrolyte additive; inorg. electrolyte solns. and gels for rechargeable lithium batteries)

IT 14024-11-4, Lithium tetrachloroaluminate 90076-65-6

RL: DEV (Device component use); USES (Uses)

(electrolyte; inorg. electrolyte solns. and gels for rechargeable lithium batteries)

IT 124-63-0, Methane sulfonylchloride 13966-08-0 14700-21-1

Trichlorophosphazosulfonyl chloride

RL: DEV (Device component use); PRP (Properties); USES (Uses)
 (solvent; inorg. electrolyte solns. and gels for rechargeable
 lithium batteries)

IT 13966-08-0 14700-21-1, Trichlorophosphazosulfonyl chloride

RL: DEV (Device component use); PRP (Properties); USES (Uses) (solvent; inorg. electrolyte solns. and gels for rechargeable lithium batteries)

RN 13966-08-0 HCAPLUS

CN Phosphorimidic trichloride, (dichlorophosphinyl) - (6CI, 8CI, 9CI) (CA INDEX NAME)

14700-21-1 HCAPLUS RN

CN Sulfamoyl chloride, (trichlorophosphoranylidene) - (7CI, 8CI, 9CI) (CA INDEX NAME)

=> => s 117-120

0 (L17 OR L18 OR L19 OR L20)

STR

=> d que

L13

-~~ N-~~ X 2 3

formula 2 187 structures from guesse

no answers

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS

STEREO ATTRIBUTES: NONE

L15 187 SEA FILE=REGISTRY SSS FUL L13 L16 96 SEA FILE=HCAPLUS ABB=ON L15

L17 0 SEA FILE=HCAPLUS ABB=ON L16(L)ELECTROLYT? L18 O SEA FILE=HCAPLUS ABB=ON L16 AND ELECTROLYT? L19 O SEA FILE=HCAPLUS ABB=ON L16 AND BATTER?

O SEA FILE=HCAPLUS ABB=ON L16 AND ELECTROCHEM?/SC,SX,AB,BI L20 0 SEA FILE=HCAPLUS ABB=ON (L17 OR L18 OR L19 OR L20)

L24

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9 AUG 2005 HIGHEST RN 859282-03-4

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=> d que 123 L13

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NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS

STEREO ATTRIBUTES: NONE

L15 187 SEA FILE=REGISTRY SSS FUL L13 L23 7 SEA FILE=REGISTRY ABB=ON L15 AND 3-15/P

=> d scan 123

7 structures with 3-15 phosphorus per claim L23 7 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN IN Iodine(1+), bis(N-iodo-P,P,P-triphenylphosphine imide- $\kappa$ N)( $\mu$ -(P,P,P-triphenylphosphine imidato-κN:κN)]di-, iodide, compd. with pentafluoroiodobenzene (1:2) (9CI) MF C54 H45 I4 N3 P3 . 2 C6 F5 I . I

CM 1

• I-

CM 2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):6

L23 7 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN Iodine(1+), bis(N-iodo-P,P,P-triphenylphosphine imide- $\kappa$ N)bis( $\mu$ -(P,P,P-triphenylphosphine imidato- $\kappa$ N: $\kappa$ N)]tri-, (triiodide) (9CI)

MF C72 H60 I5 N4 P4 . I3

CM 1

CM 2

I--I--I

L23 7 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

MF Cl12 N5 P5

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

REGISTRY COPYRIGHT 2005 ACS on STN

Iodine (1+), bis (N-iodo-P,P,P-triphenylphosphine imide- $\kappa$ N) [ $\mu$ -IN (P,P,P-triphenylphosphine imidato-κN:κN)]di-, iodide (9CI)

MF C54 H45 I4 N3 P3 . I

CCS, COM CI

7 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

Iodine (1+), bis (N-iodo-P, P, P-triphenylphosphine imide-κN) bis [μ-

(P, P, P-triphenylphosphine imidato-κN:κN)]tri- (9CI)

MF C72 H60 I5 N4 P4

CI CCS, COM

7 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN L23

Iodine(1+), bis(N-iodo-P,P,P-triphenylphosphine imide- $\kappa N$ )[ $\mu$ -

(P,P,P-triphenylphosphine imidato-κN:κN)]di- (9CI)

MF C54 H45 I4 N3 P3

CI CCS, COM

L23 7 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN

IN Phosphoramidimidic difluoride, N-[[[(difluoroamino)difluorophosphoranylide ne]amino]difluorophosphoranylidene]-N'-[N-(difluorophosphino)-P,P-

08/10/2005

RPage 29

difluorophosphinimyl] - (9CI) MF F12 N5 P5

$$F_2P-N = P-N = P-N = P-N = P-NF_2$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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2 L23

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ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN L25

AN 1999:94318 HCAPLUS

DN 130:267497

TI Domino effect in the buildup of N-I-N-I chains of the Niodine (triphenylphosphine) imine

AU Grebe, Jutta; Geiseler, Gertraud; Harms, Klaus; Neumuller, Bernhard; Dehnicke, Kurt

CS Fachbereich Chemie der Universitat, Marburg, D-35032, Germany

SO Angewandte Chemie, International Edition (1999), 38(1/2), 222-225 CODEN: ACIEF5; ISSN: 1433-7851

PB Wiley-VCH Verlag GmbH

DTJournal LA English

Depending upon the stoichiometric ratio, the reaction of Ph3PNI with iodine in CH2Cl2 gave [I(INPPh3)2]+I3- (1) and [I(INPPh3)4]+I3- (2). Reaction of INPPh3 with I2 in the presence of 1,4-diiodotetrafluorobenzene in CH2Cl2 gave [I(INPPh3)3]+[I(C6F4I2)]- (3). The crystal structure of 1-3 were determined

CC 29-7 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 75

ST nitrogen iodine chain triphenyl phosphine imine prepn structure; triphenylphosphine imine nitrogen iodine chain prepn structure; crystal mol structure nitrogen iodine chain triphenylphosphine imine

IT Crystal structure

Molecular structure

(of nitrogen iodine chain triphenylphosphine imine complexes)

IT 221354-50-3P 221354-51-4P 222412-29-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)

IT 221354-46-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and mol. structure of)

IT 392-57-4, 1,4-Diiodotetrafluorobenzene

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of iodine(triphenylphosphine)imine with iodine in presence
 of)

IT 392-57-4, 1,4-Diiodotetrafluorobenzene

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of iodine(triphenylphosphine)imine with iodine in presence
 of)

IT 221354-50-3P 222412-29-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)

RN 221354-50-3 HCAPLUS

CN Iodine(1+), bis(N-iodo-P,P,P-triphenylphosphine imide-κN)[μ-(P,P,P-triphenylphosphine imidato-κN:κN)]di-, iodide, compd. with pentafluoroiodobenzene (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 221354-49-0 CMF C54 H45 I4 N3 P3 . I CCI CCS

• I-

CM 2

CRN 827-15-6 CMF C6 F5 I

RN 222412-29-5 HCAPLUS

CN Iodine(1+), bis(N-iodo-P,P,P-triphenylphosphine imide-κN)bis[μ(P,P,P-triphenylphosphine imidato-κN:κN)]tri-, (triiodide)
(9CI) (CA INDEX NAME)

CM 1

CRN 222412-28-4 CMF C72 H60 I5 N4 P4 CCI CCS

CM 2

CRN 14900-04-0 CMF I3

#### RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1977:501818 HCAPLUS

DN 87:101818

TI Conformational analysis of phosphazenes. A force field for the calculation of the molecular structures of halophosphazenes

AU Boyd, Richard H.; Kesner, Laya

CS Dep. Mater. Sci. Eng., Univ. Utah, Salt Lake City, UT, USA

SO Journal of the American Chemical Society (1977), 99(13), 4248-56 CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

AB Phosphazenes (-N:PR2-)n are a series of compds. that include rings of various sizes and conformations and linear high-mol.-weight polymers which the formal valence structure presents the possibility of  $\pi$ -electron delocalization. An attempt was made to see if phosphazene properties could be accounted for in terms of a conventional conformational model in which the mols. are subject to the influences of the energetics of bond twisting, bending, and stretching (and nonbonded interactions), but in

which there are not further effects on bonding in various size mols. than from these sources (i.e., the individual bond energies do not depend on the size of the mol.). The geometries, energies, and vibrational frequencies of a number of cyclic perhalophosphazenes were satisfactorily accounted for by such a model. A force field for conformational calcns. on chloro- and fluorophosphazenes is presented. Important and necessary features of the model include a 2-fold torsional potential with a low barrier (.apprx.1.4 kcal/mol) and a soft bending constant at the PNP valence angle (both absolutely and relative to the NPN angle).

CC 22-9 (Physical Organic Chemistry)

ST conformation phosphazene model; force field conformation phosphazene

IT Molecular mechanics

Potential energy and function

(for calcn. of conformation of halophosphazenes)

IT Conformation and Conformers

Molecular structure

(of halophosphazenes, force-field model for calcn. of)

IT Phosphonitrile compounds

RL: PRP (Properties)

(halo, conformational anal. of, force-field model for calcn. of)

IT 940-71-6 2950-45-0 13596-41-3 14700-00-6 15599-91-4

63722-41-8 63722-42-9

RL: PRP (Properties)

(conformation of, calcn. of)

IT 63722-41-8 63722-42-9

RL: PRP (Properties)

(conformation of, calcn. of)

RN 63722-41-8 HCAPLUS

Phosphoramidimidic dichloride, [dichloro[dichloroamino]phosphora CN nylidene] amino] phosphoranylidene] [P, P-dichloro-N-(dichlorophosphino)phosphinimyl] - (9CI) (CA INDEX NAME)

RN 63722-42-9 HCAPLUS

CN Phosphoramidimidic difluoride, N-[[[(difluoroamino)difluorophosphoranylide ne] amino] difluorophosphoranylidene] -N' - [N- (difluorophosphino) -P, Pdifluorophosphinimyl] - (9CI) (CA INDEX NAME)

$$F_2P-N \longrightarrow P-N \longrightarrow P-N \longrightarrow P-N \longrightarrow P-NF_2$$